MULTIPHYSICS MODELING OF A NOVEL PHOTOELASTIC MODULATOR FOR ULTRA-HIGH PERFORMANCE FT SPECTROMETRY

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ABSTRACT

We present the multiphysics model and simulation of a virtual stack/phased array (VSPA) photoelastic modulator (PEM), a novel type of high-retardation PEM (Buican 2008) for use in ultra-high performance FT spectrometers (Buican and Carrieri 2004) with applications in the optical recognition of explosives and CB warfare agents. The multiphysics model consists mainly of coupled partial differential equations (PDE) describing a high-intensity acoustic fields driven by a phased array of attached piezoelectric transducers (PZT) and the coupled heat generation and flow driven by ultrasound absorption in the optical medium. A mixture of serial and parallel software is being used for modeling, simulation, and postprocessing. The software runs on a dedicated locally assembled PC cluster

1. INTRODUCTION

Although the bar-shaped VSPA PEM has a simple geometry, the solutions of the acoustic wave equations in the solid bar are nontrivial and analysis reveals a multitude of propagating and nonpropagating modes (Auld, 1990). Additionally, complex boundary conditions are introduced by the multiple PZTs in the phased array, together with an electromagnetic-elastic coupling in the PZTs (Auld, 1990). Furthermore, the high acoustic field amplitudes necessary in order to induce sufficient birefringence result in significant heat generation in the volume of the bar and consequent heat flow through both volume and boundary, which lead to a position- and time-dependent temperature distribution in the bar volume. The acoustic-thermal coupling loop is closed through the temperature dependence of material properties and the associated changes in the geometry of the bar, which affect elastic wave propagation and the boundary conditions themselves. The core acoustic-thermal problem is complemented by the important but simpler photoelastic coupling between elastic strain and dielectric tensor fields, and by the external electronic feedback loops that drive the array PZTs. We present in this paper a simplified version of the model describing a VSPA PEM and discuss its implementation in the COMSOL Multiphysics environment.

We briefly discuss current work aimed at interfacing the COMSOL package, which does not yet include a cluster-based solver, with high performance solvers available on the local cluster through the free Trilinos library (Heroux et al., 2003). Finally, we discuss work aimed at integrating initial model development and simulation on a small local cluster with subsequent batch processing on large shared clusters such as those at the Department of Defense Major Shared Resource Centers (MSRC). Integrated access to large clusters will be essential in the next stage of the project when device geometry and controller design will have to be optimized prior to designing a proof-of-principle prototype.

We believe that VSPA-PEM/FT spectrometry is the enabling technology for reliable real-time chemical-biological cloud detection, identification and mapping; for transient identification and mapping of RPGs; and for surface contamination detection (Buican and Carrieri, 2004, 2006, 2008). The VSPA-PEM/FT spectrometry engine can be integrated into lidars and hyperspectral imagers (Buican and Carrieri, 2008). The advanced modeling and simulation work described here is an important first step in the development of VSPA technology.

2. MULTIPHYSICS MODELING

2.1 The VSPA Concept

We have shown before (Buican and Carrieri, 2004) that photoelastic modulators (PEM) can be used use in ultra-high performance FT spectrometers with applications in the optical recognition of explosives and CB warfare agents. When used in PEM/FT spectrometers, existing PEM technologies require a compromise to be struck between spectral resolution and light throughput. This drawback can be overcome by third generation PEM/FT spectrometers based on a dedicated PEM design (VSPA) that simultaneously provides both high spectral resolution and high light throughput (Buican, 2008). The VSPA

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concept is presented in detail in our parallel paper presented at this conference (Buican and Carrieri, 2008).

The main components of a VSPA PEM are a bar-shaped optical element and the affixed array(s) of PZTs (Fig. 1).

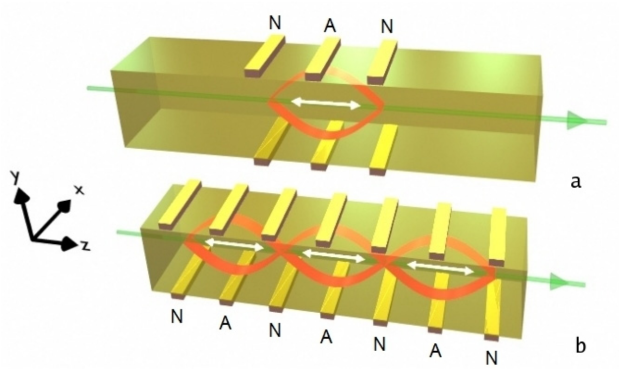

Fig. 1. The VSPA PEM optical element and attached array of PZTs. (a) Two node drivers (N) and one antinode driver (A) form an Active Resonance Cell (ARC). (b) Adjacent ARCs can share node drivers and a virtual stack of PEMs can be implemented within the bar. PZT drivers directly above each other are of the same type. Standing elastic waves are shown here by ribbon-like representations of their amplitude envelopes; white double-ended arrows represent the direction of propagation of the elastic waves; and green arrows represent the optical paths through the devices.

The basic idea behind the VSPA concept is that elastic wave propagation along the axis of the bar can be confined through the use of "active mirrors" consisting of PZTs driven at appropriate amplitudes and phases (Buican and Carrieri, 2008). Fig. 1a shows how two such active mirrors (see the parallel paper, Buican and Carrieri, 2008, for a discussion of node and antinode drivers) can be used to form an Active Resonance Cell (ARC). ARCs function like elastic wave resonators bounded by virtual reflecting surfaces; however, they have no physical discontinuities that might scatter light propagating along the axis of the bar. Furthermore, suitably driven phased arrays of PZTs placed along the PEM bar (Fig. 1b) cause the latter to behave like a stack of mechanically isolated conventional PEMs—hence the virtual-stack/phased array, or VSPA, name of the technology. Being isolated, these stacked "virtual" PEMs can be driven in phase and thus constructively contribute to a total retardation that is the scalar sum of the individual virtual PEM amplitudes. We present in the parallel paper (Buican and Carrieri, 2008) preliminary multiphysics simulation results which show that the VSPA framework does hold for a realistic 3-D VSPA system.

The VSPA design is unique because the retardation amplitude it achieves scales with bar length (and thus number of attached PZTs) while the local stress amplitude does not. This means that, within reason, the retardation amplitude can be increased simply by increasing the length of the bar and the number of PZTs without at the same time increasing internal stress amplitudes and thus compromising device reliability. The latter represents an important reliability advantage of VSPA PEMs over conventional ones. This and other reliability and cost advantages are likely to enable the development and deployment of VSPA-based compact and rugged ultra-high performance FT spectrometers for use in the field and on mobile platforms. A brief discussion of this important matter can be found in Section 5 of our parallel paper (Buican and Carrieri, 2008).

2.2 Modeling the VSPA PEM

The three main components of the VSPA multiphysics model are shown in Fig. 2. The Optical Element corresponds to the transparent bar shown in Fig.1; the PZT Array consists of PZTs like the ones shown in Fig. 1b. Finally, the Controller and Driver are a collection of digital and analog electronic circuits that monitor the currents through the various driving—and possibly sensing—PZTs and generate driving waveforms according to a response function $\mathfrak{R}$.

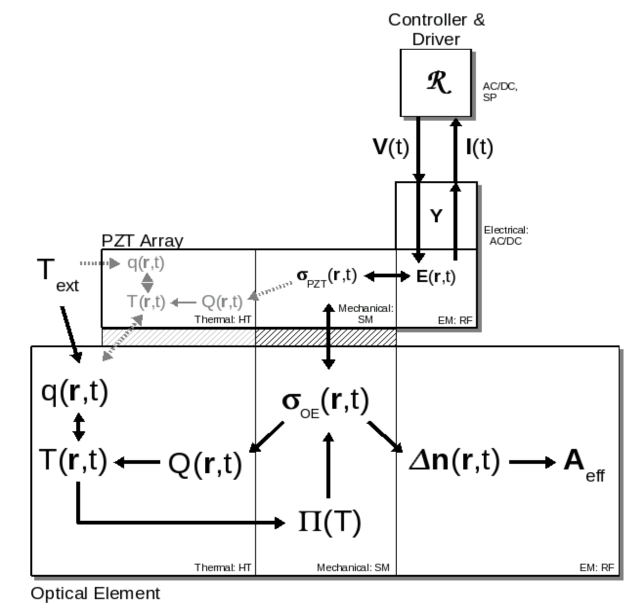

Fig. 2. Simplified diagram of the multiphysics model of a VSPA PEM, showing the three components of the model and their internal compartments. The couplings between PZT Array and Optical Element are represented by hatched areas. The internal components are labeled in the lower right corner; the included abbreviation indicates the relevant COMSOL module: AC/DC—AC/DC Module; HF—Heat Flow Module; RF: RF Module; SM—Structural Mechanics Module; SP—Signal Processing and Systems Lab. $\mathbf{A}_{eff}$—effective retardation amplitude; **E**—electric field in the PZTs ; **I**—PZT currents; $\Delta\mathbf{n}$—refractive index tensor; **q**—heat flux; Q—heat source; **r**—position vector; $\mathfrak{R}$—Controller response function; t—time; T—internal temperature; T_{ext}—external tempera-

ture; **V**—PZT driving voltages; **Y**—PZT array electrical acceptance; **Π**(T)—temperature-dependent system parameters; $\boldsymbol{\sigma}_{OE}$—stress tensor in the optical element; $\boldsymbol{\sigma}_{PZT}$—stress tensor in the PZTs. The grayed-out symbols and couplings were ignored in the initial model. (See text for details.)

The model of the optical element consists of mechanical (structural), thermal (heat transfer), and electromagnetic (optical) layers. The mechanical layer of the optical element and the corresponding layer of the PZT array model are coupled and the PZTs drive the elastic waves that propagate in the bar. The representative quantity for this layer is the stress tensor $\boldsymbol{\sigma}_{OE}(\mathbf{r},t)$ which is governed by the acoustic field PDEs (Auld, 1990, Ch.4).

The representative quantity for the thermal layer is the temperature T(**r**,t) which is governed by the heat conduction PDE (COMSOL, 2006b). The mechanical layer drives the thermal one through the volume heat source distribution Q(**r**,t) generated by stress oscillations in a lossy medium. The temperature distribution in turn affects the mechanical layer through temperature-dependent material parameters represented in Fig. 2 by Π(T). This thermal feedback loop can lead to instability in PEMs driven at high amplitudes; such instabilities can be eliminated by appropriate PZT driving control (Buican, 2006). Additionally, heat exchange with the environment contributes a heat flux term on the boundary of the optical element. Heat generation in the PZTs and heat flow between PZTs and the optical element were ignored in the initial modeling work but will be incorporated in the next version of the model.

The representative quantity for the electromagnetic (EM) layer of the Optical Element is the refractive index tensor field, $\Delta\mathbf{n}(\mathbf{r},t)$. There is a one-directional interaction from the mechanical layer to the EM one. This interaction is mediated by the stress-optical tensor (Born and Wolf, 1970, 14.5; COMSOL, 2006c, 153-185) which relates the refractive index and stress tensors. Further, the refractive index tensor determines the birefringence along an optical path and thus the effective and total retardation amplitudes (Buican and Carrieri, 2008).

As shown in Fig.2, the model of the PZT array has a mechanical layer with a stress tensor field, $\boldsymbol{\sigma}_{PZT}(\mathbf{r},t)$, which is coupled to the stress in the optical element. The thermal layer in the PZT array model has been ignored but will be included in the next version of the model. The electromagnetic layer mainly models the low-frequency electric field **E**(**r**,t) in the PZT, which is governed by Maxwell's equations (Jackson, 1998; Auld, 1990, Ch. 8). Finally, there is an electrical layer described by a generalized acceptance **Y** that relates the currents flowing through the PZTs to driving voltages.

The coupling between electric field and stress tensor in the PZTs is described by cross terms in the piezoelectric constitutive equations (Auld, 1990, 8.B; COMSOL, 2006d, 410-411). In a linear approximation, these cross terms are defined by the piezoelectric stress constant tensor. The electric field in the PZT thus couples the stress to the PZT driving voltage and current, and the mechanical response of the VSPA PEM to the PZT array electrical acceptance. The latter coupling allows the external controller not only to monitor the instantaneous state of the PEM, but also to fine-tune its dynamic behavior (Buican, 2006).

2.3 Multiphysics Modeling

The Finite Element Method (FEM) (Braess, 2001; Pepper and Heinrich, 2006; COMSOL, 2006a) is a numerical technique for solving partial differential equations by discretizing their spatial domain into a mesh of small but arbitrarily shaped regions (finite elements). This results in matrix equations that relate the input at certain points (nodes) in the elements to outputs at the same points. Several well-established commercial packages based on FEM algorithms are available.

For this work, we chose COMSOL Multiphysics (COMSOL, 2006a) because of its ease of use and flexibility in incorporating and integrating models for a multitude of interacting physical phenomena. Through COMSOL Script (see below), COMSOL Multiphysics also provides the user with fairly easy access to internal model data. As discussed in Subsection 2.2, the VSPA model includes several types of interacting physical phenomena, each described by its own PDEs: (1) continuum mechanics/elasticity/acoustics; (2) electromagnetism, both low-frequency (PZT drivers) and high-frequency (optical element); and (3) heat flow. Additionally, the VSPA model includes (4) AC electrical circuits; and (5) signal processing. These five interacting model layers map directly to COMSOL Multiphysics modules: (1) Structural Mechanics; (2) RF; (3) Heat Transfer; (4) AC/DC; and (5) Signals & Systems Lab. Beyond these modules, COMSOL Script adds a Matlab-like scripting language that we have used extensively (see the discussion of the SEAMPHYS interface to COMSOL in Section 3.1.), as well as Optimization Lab, which will allow us to optimize VSPA model parameters.

Preliminary modeling results for the VSPA model are presented in Subsection 4.1 of our parallel paper (Buican and Carrieri, 2008).

3. COMPUTATION

3.1 Modeling and Data Processing Software

We are currently using both free open-source and commercial off-the-shelf (COTS) finite element modeling (FEM) software to create comprehensive multiphysics models of the VSPA PEM optical element. The models are developed and tested on HERD-0, a small in-house PC cluster (see below).

The basic modeling package used in this work was COMSOL Multiphysics Version 3.4. The Multiphysics framework was supplemented by COMSOL modules for modeling the mechanical, thermal, and electromagnetic processes in the PEM bar and PZT array, as well as the system controller/driver.

Version 3.4 of COMSOL includes the Pardiso solver (Schenk and Gärtner, 2004), which makes use of shared-memory parallelism but not of cluster-based distributed-memory parallelism. (It should be noted that the just-released version 3.5 of COMSOL reportedly can use cluster-based parallelism for its parametric solver—the quintessential "embarrassingly parallel problem" described by Foster, 1995). Thus, solver performance for the available COMSOL package could only be improved by replacing, rather than extending, the hardware platform. As explained in the next Subsection, PC clusters offer important advantages in terms of cost, flexibility, and availability of high-performance computing (HPC) capabilities. We therefore decided to use cluster-based solvers in our modeling work, both on our own small cluster, HERD-0, and on jvn, a larger cluster at the Army Research Laboratory's (ARL) MSRC. We also decided to use Trilinos (Heroux et al., 2003), a very capable free library of object-oriented linear algebra tools and solvers designed for use on clusters.

We developed in house a Trilinos-based solver that includes a COMSOL Multiphysics interface (Fig. 3).

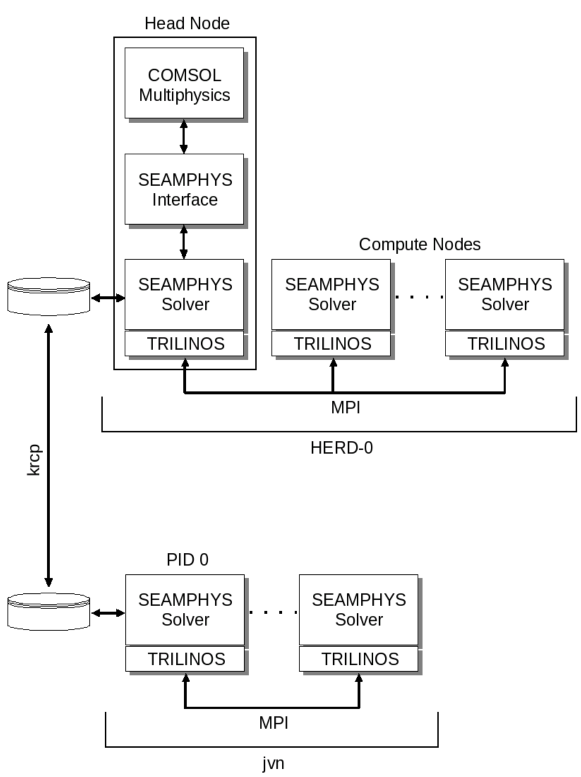

Fig. 3. SEAMPHYS installation on the local cluster HERD-0 (top) and the ARL MSRC cluster "jvn" (bottom). MPI—Message-Passing Interface; krcp—Kerberos-based remote file copy; PID 0—MPI process with ID 0. (See text for explanation.)

This package, dubbed SEAMPHYS, allows a model set up in COMSOL to be transferred, via COMSOL Script (COMSOL AB, 2006a), Java/JNI and C++ code, to the appropriate cluster-based Trilinos solvers, and the results transferred back to COMSOL for postprocessing and display. At this time, two linear solver packages available through the Trilinos library, Amesos (Sala and Stanley, 2004) and AztecOO (Heroux, 2004), have been successfully used to solve COMSOL Multiphysics problems. We plan to add access to the Anasazi eigensolver (Baker et al., 2008) in the near future.

The structure and use of the SEAMPHYS package are illustrated in Fig.3. COMSOL Multiphysics and the SEAMPHYS interface run on the head node of the local cluster, while the SEAMPHYS solver can run in parallel on all HERD-0 nodes and on jvn nodes. At this time, the local and remote clusters exchange data through files transferred via the internet through Kerberos-based remote copy, krcp. The SEAMPHYS solver modules use the Trilinos library solvers, as well as the MPI-based (Snir et al., 1998) interprocess communication capabilities encapsulated in the Trilinos C++ classes. Tests of the SEAMPHYS solver installed on jvn are currently under way.

3.2 High-Performance Data Processing

The ability of PC clusters to provide improved performance simply through the addition of inexpensive, commodity-grade hardware is very attractive. When complemented by the availability of very capable and free cluster management software and cluster-ready solvers, PC clusters are the solution of choice where flexible and low-cost high-performance computing (HPC) capabilities are required.

The HERD-0 cluster (Fig. 4) was assembled at SEA LLC for initial physical modeling work. Each of the nine nodes has a dual-core Athlon 64 processor and 3 GB of RAM. The nine PCs are connected by a private Gigabit Ethernet network and are powered by uninterruptible power supplies. HERD-0 exceeded 56 Gflops.

The HERD-0 cluster uses many freely available, open-source software packages such as the Rocks cluster management

Fig. 4. The HERD-0 PC cluster.

system (Papadopoulos et al., 2001), GNU compilers (gcc.gnu.org, 2008), OpenMPI libraries (open-mpi.org, 2008) and other MPI implementations, and the Trilinos library of object-oriented linear algebra tools and solvers (Heroux et al., 2003).

Once a model has been developed and debugged on HERD-0, production runs will be carried out on jvn (arl.hpc.mil, 2008), a Linux Networx Evolocity II PC cluster at the ARL MSRC, Aberdeen Proving Ground, MD. Jvn has 2,048 Intel Xeon EM64T processors with a clock speed of 3.6 GHz and a total of 4 TB of RAM. Jvn employs a high speed Myrinet interconnect and can reach 14.7 TFlops.

We would like to point out that our approach to using HPC could be generalized for use in many small-scale research projects carried out by small teams. Indeed, HPC adoption by small research teams with small budgets is difficult, in part, because it requires a considerable initial investment of time and funds as models are slowly developed and debugged on large remote PC clusters at shared resources. Our approach, which consists of (1) assembling a small and inexpensive but very capable local PC cluster for quick model development and debugging, and (2) using software tools that transparently move data and solver execution from the local to the remote cluster for production runs, could be developed into a ready-to-use and generally available software and documentation package.

CONCLUSIONS

Our initial multiphysics modeling work shows that the VSPA concept holds considerable promise as the basis for high retardation amplitude PEMs for use in ultra-high performance FT spectrometers. Furthermore, the results of the theoretical, modeling and data processing work performed so far place us in a strong position to carry out improved modeling and, most importantly, direct experimental work on the VSPA technology, with a view to designing and assembling a technology prototype.

We believe that VSPA PEM/FT spectrometry has the potential to become the enabling technology for fast, sensitive, and reliable optical detection and identification of trace amounts of explosives, as well as chemical and biological agents and contaminants.

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